UC SANTA BARBARA

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Revolutionizing Polymer Simulation

For 15 years, Glenn H. Fredrickson and his collaborators have been building computer models for the interaction of polymer building blocks. The materials researchers have developed a method that enables rapid simulations of highly complex polymer systems, which vastly expands the number of “recipes” that can be tried.

“People modify the chemical structure of the building blocks and the monomers that make up the polymers,” explained Fredrickson, a professor in UC Santa Barbara’s Department of Chemical Engineering and the campus’s Materials Research Laboratory. “There are multiple components, and how they all interact to establish material properties is generally determined in an Edisonian trial-and-error kind of way.

“We dreamed that we could build computer models for how all these components interact, and then run some sort of simulation to see how the material would structure and what its properties might be,” Fredrickson added. “The system requires a feedback loop so that multiple computers can grind away trying to determine an optimal recipe.”

Fredrickson and his collaborators have realized that dream — and earned widespread recognition for their revolutionary accomplishments, which altogether play a critical role in developing new polymers to support the ongoing micro-electronics revolution. Among the honors Fredrickson has received is the American Institute of Chemical Engineers William H. Walker Award for Excellence in

Contributions to Chemical Engineering Literature. Coming more recently, the Materials Research Society's Materials Theory Award cited him for "pioneering the development of field-theoretic computer simulation methods and their application to investigate and design self-assembling polymers and soft material."

"This award recognizes Glenn Fredrickson's immense and impactful contributions to theory and simulation of polymer self-assembly," said Rachel Segalman**,** the Edward Noble Kramer Professor and chair of UCSB's Department of Chemical Engineering. "Many of the methods Glenn has developed are now widely used both in academia and in industrial systems. We are incredibly proud of his achievements."

"We're trying to develop new ways of simulating soft materials — complex materials composed of polymers and other ingredients, which can be applied in developing new types of plastics as well as consumer products," said Frederickson.

The challenge in simulating polymers of practical interest as materials is that they are usually very large macromolecules. When they are melted together, their entangled chains resemble spaghetti, and because they are so entangled, they move very slowly.

"It's easy to do a molecular simulation of a small, relatively simple molecule like water, but when you have a highly concentrated assembly of polymers, the constituent parts barely move, and you end up being limited by the time scale of the simulation you can run," Fredrickson noted. "In most cases, even with massive computer resources, it's not possible to run simulations long enough to bring such a system to an equilibrium state in which the material structure is established and properties don't change."

Fredrickson's lab came up with a revolutionary alternative that transformed the many-polymer model into a field theory. This approach allowed the researchers to equilibrate very dense polymer systems that have high molecular weight and are structured on length scales ranging from nanometers to microns. With that ability, they can pursue a vast range of applications.

This "field-theoretic simulation" (FTS) approach is significant not only for its fundamental importance to polymer science and molecular thermodynamics, but also for its engineering impact on directed self-assembly, an emerging lithographic technique for patterning semiconductor devices. Companies such as Intel and Samsung are developing next-generation lithographic processes based on FTS

software tools developed by the Fredrickson group at UCSB. Now, the industry challenge is to move to a finer and finer scale.

According to Fredrickson, one of the biggest hurdles is avoiding defects, which need to be reduced to the parts-per-billion level. “This is an industry that doesn’t like defects, and self-assembling soft materials are intrinsically defective,” he said. “So, with our corporate partners, we have exploited the FTS modeling tools to better understand the types of defects that occur and to help them design directed self-assembly processes that minimize defect formation.”

About UC Santa Barbara

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